Quantum Description of NMR

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Outline

History of NMR

- 1938 Prof. Rabi, First detection of nuclear magnetic spin (1944 Nobel prize)
- 1946 Prof. Purcell, Torrey, Pound, detected signals in Paraffin.

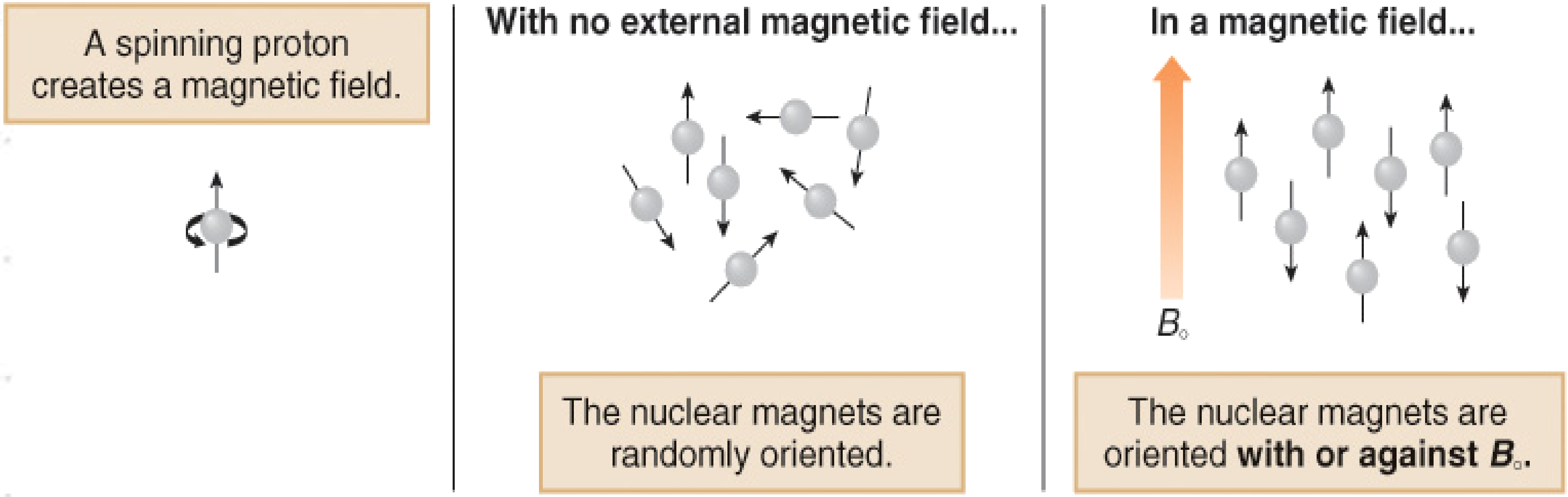
  Prof Bloch, Hansen, Packard, detected signals in water

  (Purcell, Bloch, 1952 Nobel Prize)
- 1950 Prof. Haln, Discovery of spin echo.

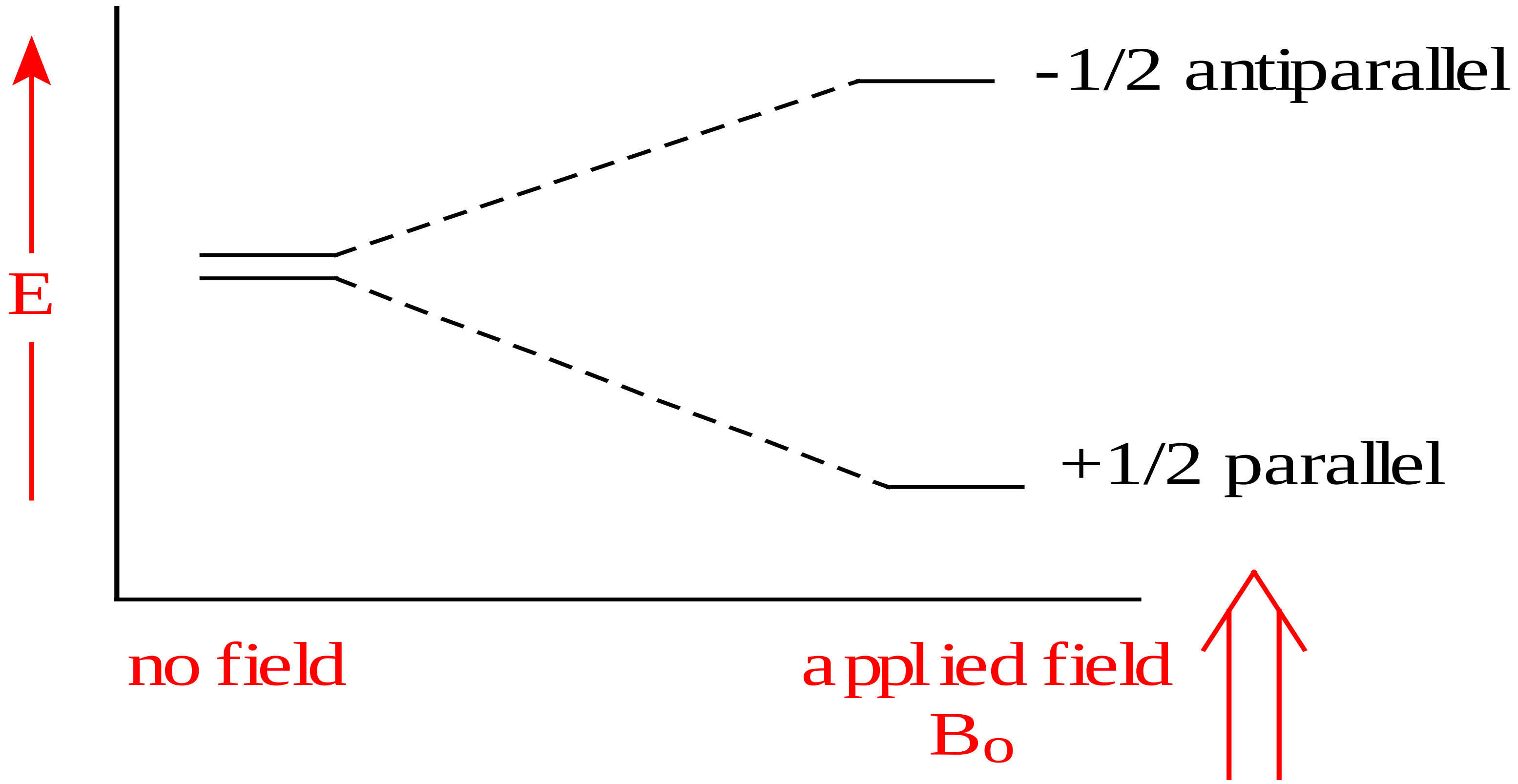
NMR

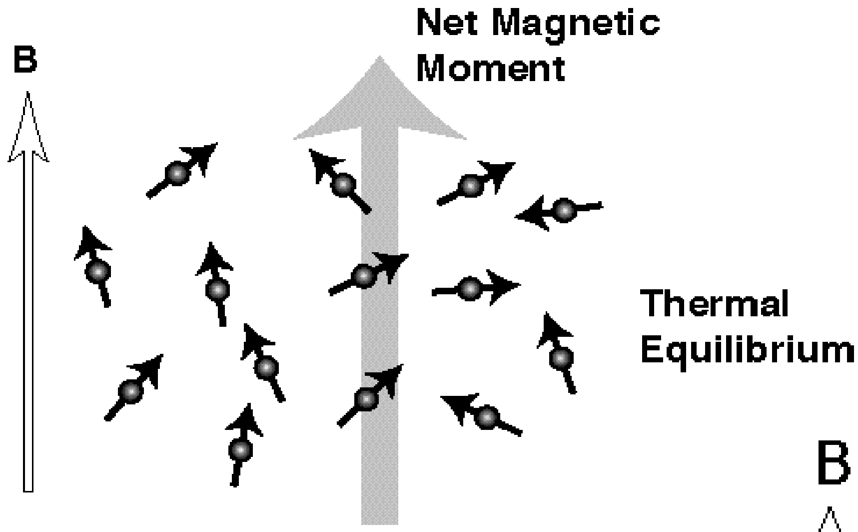
- NMR is a phenomenon in which the resonance frequencies of nuclear magnetic systems are investigated.
- NMR always employs some form of magnetic field (usually a strong externally applied field B_0)
- NMR is a form of both absorption and emission spectroscopy, in which resonant radiation is absorbed by an ensemble of nuclei in a sample.

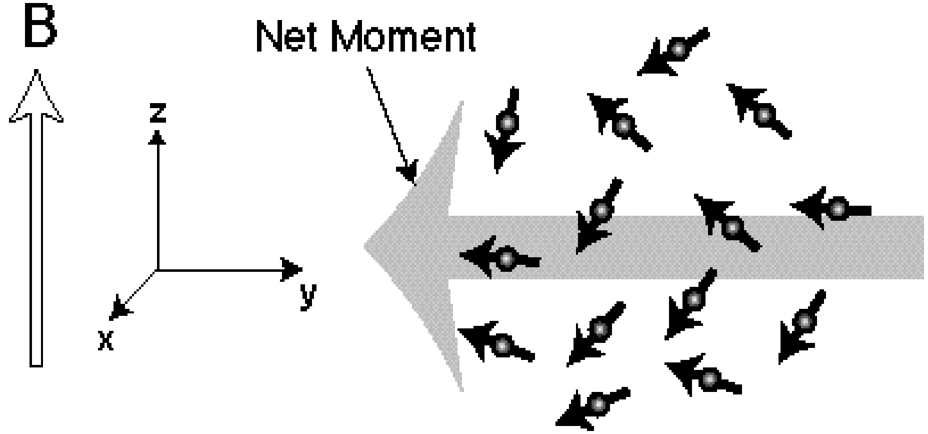
View


A spinning proton creates a magnetic field.
With no external magnetic field...
The nuclear magnets are randomly oriented.
In a magnetic field...
B_0
The nuclear magnets are oriented **with or against B_0.**

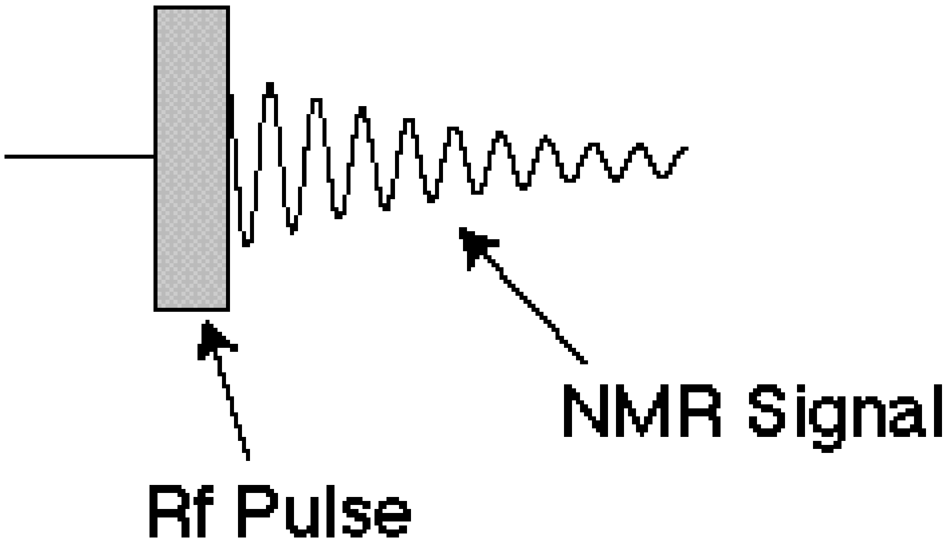
Spin States Split in the presence of $\mathbf{B_0}$




Net Magnetic
Moment
B
Thermal
Equilibrium


B
Net Moment
z
y
x

Signal Obtained



Information from NMR spectra of e.g for Hydrogen

1. Number of signals: How many different types of hydrogens in the molecule.
2. Position of signals (chemical shift): What types of hydrogens.
3. Relative areas under signals (integration): How many hydrogens of each type.
4. Splitting pattern: How many neighboring hydrogens.

Applications of NMR

- Physics
  - Condensed matter physics
- Chemistry
  - Identification of material
- Biophysics
  - Analysis of Protein structure
- Medical
  - MRI (Magnetic Resonance Image)

Most commonly studied nuclei

Spin-1/2 nucleus	NMR freq (at 10 T)	abundance
^{1}H	426 MHz	99.9%
^{13}C	107	1.1%
^{15}N	43	0.4%
^{19}F	401	100%
^{28}Si	85	4.7%
^{31}P	175	100%

Quantum Mechanical Description

- The Spin Magnetic Moment and Spin Angular Momentum are related by

$$\mu = \gamma \mathrm{I}$$

- When placed in Magnetic Field this magnetic moment has energy E.

$$E = -\mu \cdot \mathrm{B}$$

- Spin Hamiltonian

$$H = -\gamma \hbar \mathrm{B} \cdot \mathrm{I}$$

- If B is applied along z-axis then H is called as Zeeman Hamiltonian

$$H = -\gamma \hbar B_z I_z$$

- Eigenvalue equations for spin-1/2 along x, y and z-axis are

$$I_z|\uparrow\rangle = +1/2|\uparrow\rangle \qquad I_z|\downarrow\rangle = -1/2|\downarrow\rangle$$

$$I_x|\uparrow\rangle = +1/2|\downarrow\rangle \qquad I_x|\downarrow\rangle = -1/2|\uparrow\rangle$$

$$I_y|\uparrow\rangle = +1/2i|\downarrow\rangle \qquad I_y|\downarrow\rangle = -1/2i|\uparrow\rangle$$

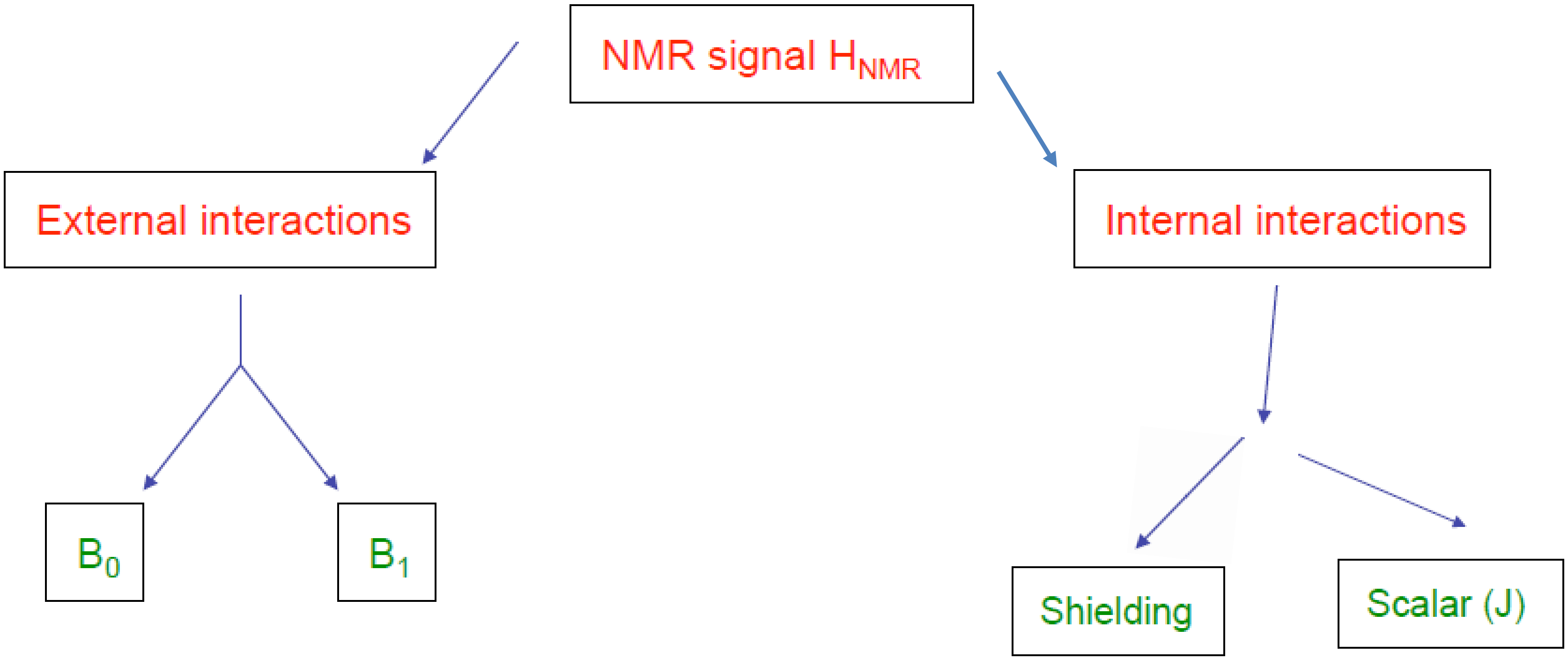
Matrix Representation

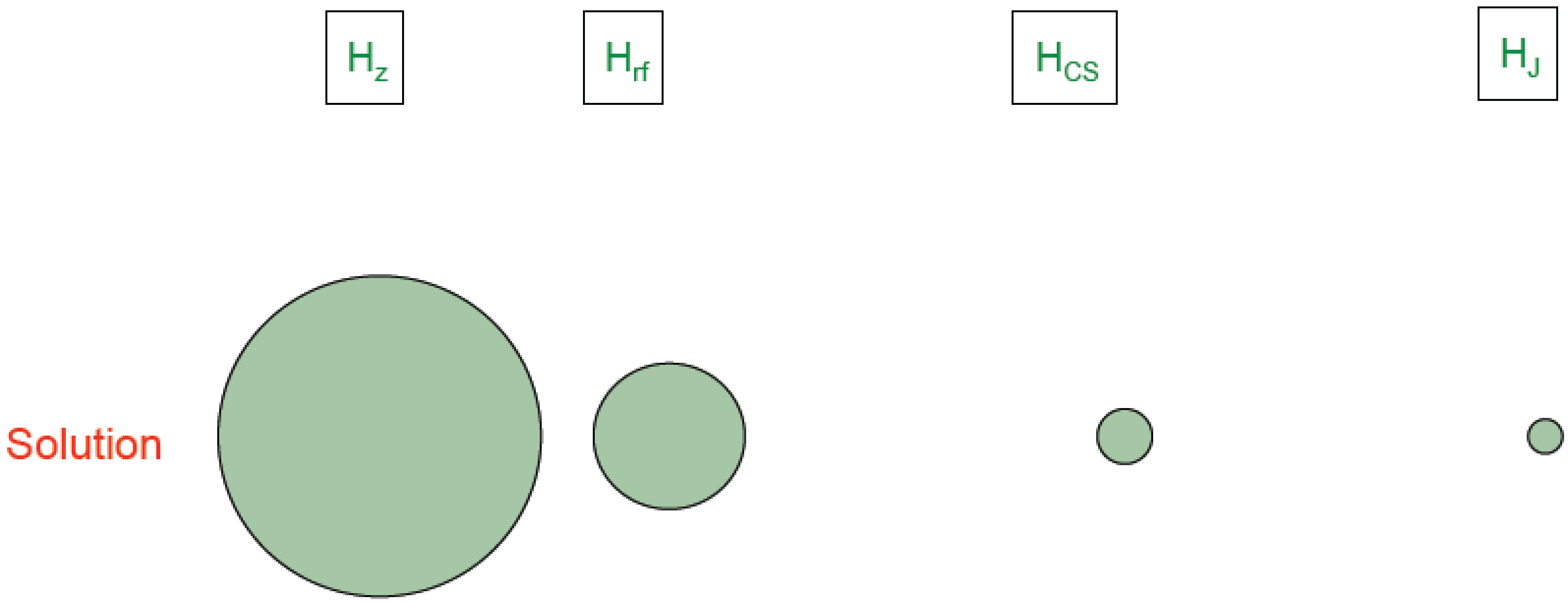
- Using ‘ $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ ‘ Up state
- ‘ $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$‘ Down state

$$I_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad I_y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$I_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Interactions in NMR




H_z
H_{rf}
H_{CS}
H_J
Solution

Total Hamiltonian

- Static Magnetic Field

$$\mathrm{B}_0 = B_z \hat{k}$$

- Radio-Frequency Field

$$\mathrm{B}_1(t) = B_1 \cos(\omega_0 t + \phi)\hat{i} - B_1 \sin(\omega_0 t + \phi)\hat{j}$$

- Total H will become

$$H = \omega_0 I_z + \omega_1 (I_x \cos(\omega_0 t + \phi) - I_y \sin(\omega_0 t + \phi))$$

- Where

$$\omega_0 = -\gamma B_z \bullet\ , \quad \omega_1 = -\gamma B_1$$

- Transformation propagator

$$U = \exp(i\omega_0 t\, I_z)$$

- Hamiltonian transforms to

$$H' = U H U^{-1} + i\dot{U} U^{-1}$$

$$H' = \omega_1 (I_x \cos\phi + I_y \sin\phi)$$

- Take $\phi = 0$

$$H' = \omega_1 I_x$$

Density Matrix Formalism

- A tool used to describe the state of a spin ensemble, as well as its evolution in time.

$$\rho = |\downarrow\rangle\langle\downarrow|$$

- Average of any observable

$$\langle A \rangle = \mathrm{Tr}(\rho A)$$

For an arbitrary state $c_\uparrow|\uparrow\rangle + c_\downarrow|\downarrow\rangle$,

Diagonal elements = probabilities

$$\rho = \begin{pmatrix} c_\uparrow^* & c_\downarrow^* \end{pmatrix} \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix} = \begin{pmatrix} |c_\uparrow|^2 & c_\downarrow^* c_\uparrow \\ c_\uparrow^* c_\downarrow & |c_\downarrow|^2 \end{pmatrix}$$

Off-diagonal elements = "coherences"
(provide info. about relative phase)

My Research Work

- After study of operators in Hilbert Space.
- Study of Superoperators in Liouville Space
- Study the classes of Decomposable and Non-decomposable Superoperators.
- Plan to simulate the unitary or non-unitary evolution of NMR states described by Superoperators in Mathamatica.
- Will simulate various QIP processes by using superoperators.

- Liouville-von Neumann equation

$$i\hbar \frac{d\rho}{dt} = [H, \rho]$$

- We define a superoperator

$$\hat{\hat{L}}|\rho(t)\rangle = |[H, \rho(t)]\rangle$$

$$i\hbar \frac{d|\rho(t)\rangle}{dt} = \hat{\hat{L}}|\rho(t)\rangle$$

Table

Name	Continuous representation	Continuous scalar product	Discrete representation	Discrete scalar product
Superoperator space	superoperators	$\sum_{\hat{M}} \langle \hat{M} \| \hat{\hat{P}}^{\dagger} \hat{\hat{Q}} \| \hat{M} \rangle$	*$n^2 \times n^2$ matrices*	$\mathrm{Tr}\left(P^{\dagger} Q \right)$
Liouville space	operators, Density matrices	$\sum_{\varphi} \langle \varphi \| \hat{M}^{\dagger} \hat{K} \| \varphi \rangle$	*$n \times n$ matrices*	$\mathrm{Tr}\left(M^{\dagger} N \right)$
Hilbert space	wavefunctions	$\int \varphi^{*}(x) \psi(x)\, dx$	*n -vectors*	$\sum_{n} \varphi_n^{*} \psi_n$

Why NMR?

A major requirement of a quantum computer is that the coherence should last long.

> Nuclear spins in liquids retain coherence ~ 100's millisec and their longitudinal state for several seconds.

> A system of N coupled spins (each spin 1/2) form an N qubit Quantum Computer.

> Unitary Transform can be applied using R.F. Pulses and various logical operations and quantum algorithms can be implemented.

References

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- *Mayne C.L*, **Liouville Equation of Motion**, Encycl. Nucl. Mag. Res, 2717-2730.
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THANKS FOR YOUR PATIENCE